ELSEVIER

Chemical Physics 185 (1994) 414–417

Chemical Physics

Author index to volume 185

Baer, B.J. and E.L. Chronister, Inhomogeneous spectral broadening in pentacene doped para-terphenyl crystals at high pressure and low temperature 185 (1994) 385
Bagnich, S.A., Triplet excitation migration for compound molecules in solid solutions 185 (1994) 229
Barzoukas, M., A. Fort, P. Boy, C. Combellas and A. Thiebault, Experimental and computational investigation of the quadratic hyperpolarizability of a series of diaryls and polyaryls 185 (1994) 65
Bäuerle, P., see M. Bennati 185 (1994) 221
Bauschlicher Jr., C.W., see M. Sodupe 185 (1994) 163
Bednarek, G., R.P. Wayne, J. Wildt and E.H. Fink, The yield of $O_2(b\ ^1\Sigma_g^+, v=0)$ produced by quenching of $O_2(A\ ^3\Sigma_u^+, v=8)$ by O_2 185 (1994) 251
Bendazzoli, G.L., see S. Evangelisti 185 (1994) 47
Benderskii, V.A., S.Yu. Grebenshchikov, D.E. Makarov and E.V. Vetoshkin, Tunneling trajectories of two-proton transfer 185 (1994) 101
Bennati, M., A. Grupp, P. Bäuerle and M. Mehring, Pulsed-EPR on the photoexcited triplet state of C_{60} in fluid solution: electron transfer from end-capped quaterthiophene and C_{60}-radical anion formation 185 (1994) 221
Billing, G.D., see M.B. Sevryuk 185 (1994) 199
Bisht, P.B., see D.D. Pant 185 (1994) 137
Bouteiller, Y., see P. Pullumbi 185 (1994) 13
Bouteiller, Y., see P. Pullumbi 185 (1994) 25
Boy, P., see M. Barzoukas 185 (1994) 65
Buenker, R.J., see J. Gu 185 (1994) 39
Buján-Núñez, M.C. and M.A. López-Quintela, Fractal approach to the kinetics of an encounter pair between asymmetric reagents 185 (1994) 211

Carey, M.J. and D. Phillips, Modelling excimer formation in vinyl aromatic polymers 185 (1994) 75
Chibotaru, L.F. and I.N. Kotov, Polaron-like variational solutions for low-lying vibronic states 185 (1994) 153
Chronister, E.L., see B.J. Baer 185 (1994) 385
Clary, D.C., see A.G. Wickham 185 (1994) 57
Combellas, C., see M. Barzoukas 185 (1994) 65
Coplan, M.A., see C.K. Subramaniam 185 (1994) 237

De Saxce, A., N. Sanna, A. Schriver and L. Schriver-Mazzuoli, Matrix isolation investigation of the vibrational spectroscopy and photochemistry of complexes of HCl and HBr with nitric oxide. Ab initio study of the NO:HCl complex structure 185 (1994) 365

Doetschman, D.C., D.W. Dwyer, J.D. Fox, C.K. Frederick, S. Scull, G.D. Thomas, S.G. Utterback and J. Wei, Physical characterization of the state of motion of the phenalenyl spin probe in cation-exchanged faujasite zeolite supercages with pulsed EPR 185 (1994) 343
Doktorov, A.B., see A.M. Osintsev 185 (1994) 281
Dwyer, D.W., see D.C. Doetschman 185 (1994) 343

Elofson, P.A., see E. Wallin 185 (1994) 91
Evangelisti, S., G.L. Bendazzoli and L. Gagliardi, Full configuration interaction calculations on Be_2 185 (1994) 47

Fehér, M., A. Rohrbacher and J.P. Maier, Infrared laser kinetic spectroscopy of the H_3^+ ion 185 (1994) 357
Felder, P. and G.P. Morley, Photodissociation of ClNO in the A band 185 (1994) 145
Ferrari, L., The evolution of simple velocity averages of ions in gases in time-varying electric fields and static magnetic fields 185 (1994) 179
Fink, E.H., see G. Bednarek 185 (1994) 251
Fort, A., see M. Barzoukas 185 (1994) 65
Fox, J.D., see D.C. Doetschman 185 (1994) 343
Frederick, C.K., see D.C. Doetschman 185 (1994) 343

Gagliardi, L., see S. Evangelisti 185 (1994) 47
Grebenshchikov, S.Yu., see V.A. Benderskii 185 (1994) 101
Grupp, A., see M. Bennati 185 (1994) 221
Gu, J., R.J. Buenker and G. Hirsch, Ab initio CI study of the electronic spectrum of the interstellar free radical CP 185 (1994) 39
Gupta, N. and K.S.V. Santhanam, Chemiluminescent electron transfer reactions of C_{60} anion radical: energetics and spectral features 185 (1994) 113
Gürtler, P., see A.V. Kanaev 185 (1994) 129

Hirsch, G., see J. Gu 185 (1994) 39
Holmlid, L., see E. Wallin 185 (1994) 91

Jedlovszky, P., see G. Pálinkás 185 (1994) 173
Joshi, H.C., see D.D. Pant 185 (1994) 137
Joyeux, M., Semiclassical quantization of the spectroscopist's Hamiltonian for coupled vibrational modes 185 (1994) 263

Kanaev, A.V., T. Möller and P. Gürtler, Time-resolved spectroscopy of gaseous xenon excited in the vicinity of the first resonance line 185 (1994) 129
Kotov, I.N., see L.F. Chibotaru 185 (1994) 153
Kowari, K. and B.D. Shizgal, Electron degradation and thermalization in SiH_4 gas 185 (1994) 1
Kuznetsov, An.M. and W. Lorenz, Quantum-chemical ab initio investigation of the two-step charge transfer process of hydrogen reaction: approach of reaction pathways via a hydrogen intermediate on Cu(100) 185 (1994) 333

Lee, S., see J. Sung 185 (1994) 413
Leung, K.T., see C.K. Subramaniam 185 (1994) 237
Li, W., see C.-K. Zhang 185 (1994) 309

López-Quintela, M.A., see M.C. Buján-Núñez 185 (1994) 211
Lorenz, W., see An.M. Kuznetsov 185 (1994) 333

Maier, J.P., see M. Fehér 185 (1994) 357
Makarov, D.E., see V.A. Benderskii 185 (1994) 101
Manceron, L., see P. Pullumbi 185 (1994) 13
Manceron, L., see P. Pullumbi 185 (1994) 25
Mehring, M., see M. Bennati 185 (1994) 221
Mijoule, C., see P. Pullumbi 185 (1994) 13
Mijoule, C., see P. Pullumbi 185 (1994) 25
Möller, T., see A.V. Kanaev 185 (1994) 129
Moore, J.H., see C.K. Subramaniam 185 (1994) 237
Moore, J.H., see J.A. Tossell 185 (1994) 297
Morley, G.P., see P. Felder 185 (1994) 145
Muller, J.M., E.E. van Faassen and G. van Ginkel, Experimental support for a novel compound motion model for the time-resolved fluorescence anisotropy decay of TMA-DPH in lipid vesicle bilayers 185 (1994) 393

Nakagaki, R., Comment on "Photochemical reaction of 4-methyl-2-quinolinecarbonitrile with optically active (S)- or (R)-2-phenylpropionic acid. The magnetic-field and solvent effects and chiral-symmetry breaking" 185 (1994) 405

Osherov, V.I., L.V. Poluyanov, V.G. Ushakov and A.I. Voronin, Quantum scattering on the Σ–Π intersection of potential energy surfaces 185 (1994) 123
Osintsev, A.M., P.A. Purtov and A.B. Doktorov, Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. IV. Stimulated polarization of nuclei in switched external magnetic field 185 (1994) 281

Pálinkás, G. and P. Jedlovszky, Network of strongly interacting atoms in liquid argon 185 (1994) 173
Pant, D.D., H.C. Joshi, P.B. Bisht and H.B. Tripathi, Dual emission and double proton transfer in salicylic acid 185 (1994) 137
Phillips, D., see M.J. Carey 185 (1994) 75
Poluyanov, L.V., see V.I. Osherov 185 (1994) 123
Pullumbi, P., C. Mijoule, L. Manceron and Y. Bouteiller, Aluminium, gallium and indium dihydrides. An IR matrix isolation and ab initio study 185 (1994) 13
Pullumbi, P., Y. Bouteiller, L. Manceron and C. Mijoule, Aluminium, gallium and indium trihydrides. An IR matrix isolation and ab initio study 185 (1994) 25
Purtov, P.A., see A.M. Osintsev 185 (1994) 281

Ren, T.-Q., see C.-K. Zhang 185 (1994) 309
Rohrbacher, A., see M. Fehér 185 (1994) 357
Rösch, N., see I. Wilhelmy 185 (1994) 317

Sanna, N., see A. de Saxce 185 (1994) 365
Santhanam, K.S.V., see N. Gupta 185 (1994) 113
Schriver, A., see A. De Saxce 185 (1994) 365
Schriver-Mazzuoli, L., see A. De Saxce 185 (1994) 365

Scull, S., see D.C. Doetschman 185 (1994) 343
Sevryuk, M.B. and G.D. Billing, Vibrational transition probabilities for the CO molecule trapped in an argon cluster: a semiclassical simulation 185 (1994) 199
Shin, K.J., see J. Sung 185 (1994) 413
Shizgal, B.D., see K. Kowari 185 (1994) 1
Sodupe, M. and C.W. Bauschlicher Jr., A study of the ground and low-lying states of $MgC_2H_2^+$ and $MgC_2H_4^+$ 185 (1994) 163
Subramaniam, C.K., M.A. Coplan, J.A. Tossell, J.H. Moore and K.T. Leung, (e, 2e) Momentum spectroscopic study of the valence orbitals of hydrogen selenide 185 (1994) 237
Sung, J., K.J. Shin and S. Lee, Theory of diffusion-influenced fluorescence quenching. Effects of static quenching on the Stern–Volmer curve (Chemical Physics 167 (1992) 17–36). Erratum 185 (1994) 413

Thiebault, A., see M. Barzoukas 185 (1994) 65
Thomas, G.D., see D.C. Doetschman 185 (1994) 343
Tossell, J.A., see C.K. Subramaniam 185 (1994) 237
Tossell, J.A., D.C. Winkler and J.H. Moore, The lowest energy unoccupied molecular orbitals of the cyclopolysilanes: experimental and theoretical studies 185 (1994) 297
Tripathi, H.B., see D.D. Pant 185 (1994) 137

Ushakov, V.G., see V.I. Osherov 185 (1994) 123
Utterback, S.G., see D.C. Doetschman 185 (1994) 343

Van Faassen, E.E., see J.M. Muller 185 (1994) 393
Van Ginkel, G., see J.M. Muller 185 (1994) 393
Vetoshkin, E.V., see V.A. Benderskii 185 (1994) 101
Voronin, A.I., see V.I. Osherov 185 (1994) 123

Wallin, E., P.A. Elofson and L. Holmlid, Rotational surprisals and energy disposal from statistical simulations of the crossed beam reaction $C(^3P)+NO\rightarrow CN(v)+O(^3P)$ 185 (1994) 91
Wayne, R.P., see G. Bednarek 185 (1994) 251
Wei, J., see D.C. Doetschman 185 (1994) 343
Wickham, A.G. and D.C. Clary, Calculation of product branching ratios for the reaction of an ion with a molecule in a $^2\Pi$ electronic state 185 (1994) 57
Wildt, J., see G. Bednarek 185 (1994) 251
Wilhelmy, I. and N. Rösch, Molecular photoionization cross sections by the Lobatto technique. II. Core level photoionization 185 (1994) 317
Winkler, D.C., see J.A. Tossell 185 (1994) 297

Zhang, C.-K., T.-Q. Ren, W. Li and Y.-C. Zhang, Improved sudden and adiabatic nuclei theories of atom–diatomic molecule scattering 185 (1994) 309
Zhang, Y.-C., see C.-K. Zhang 185 (1994) 309

ELSEVIER

Chemical Physics 185 (1994) 418–427

Chemical Physics

Subject index to volume 185

Methods

Theoretical

Classical mechanics

Semiclassical quantization of the spectroscopist's Hamiltonian for coupled vibrational modes, M. Joyeux 185 (1994) 263

Coupling schemes and perturbative treatments

Polaron-like variational solutions for low-lying vibronic states, L.F. Chibotaru and I.N. Kotov 185 (1994) 153

Transport quantum mechanics

Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. IV. Stimulated polarization of nuclei in switched external magnetic field, A.M. Osintsev, P.A. Purtov and A.B. Doktorov 185 (1994) 281

Non-equilibrium thermodynamic and hydrodynamic theories

Electron degradation and thermalization in SiH_4 gas, K. Kowari and B.D. Shizgal 185 (1994) 1
The evolution of simple velocity averages of ions in gases in time-varying electric fields and static magnetic fields, L. Ferrari 185 (1994) 179

Ab initio schemes for stationary properties

Aluminium, gallium and indium dihydrides. An IR matrix isolation and ab initio study, P. Pullumbi, C. Mijoule, L. Manceron and Y. Bouteiller 185 (1994) 13
Aluminium, gallium and indium trihydrides. An IR matrix isolation and ab initio study, P. Pullumbi, Y. Bouteiller, L. Manceron and C. Mijoule 185 (1994) 25
Ab initio CI study of the electronic spectrum of the interstellar free radical CP, J. Gu, R.J. Buenker and G. Hirsch 185 (1994) 39
Full configuration interaction calculations on Be_2, S. Evangelisti, G.L. Bendazzoli and L. Gagliardi 185 (1994) 47
A study of the ground and low-lying states of $MgC_2H_2^+$ and $MgC_2H_4^+$, M. Sodupe and C.W. Bauschlicher Jr. 185 (1994) 163
The lowest energy unoccupied molecular orbitals of the cyclopolysilanes: experimental and theoretical studies, J.A. Tossell, D.C. Winkler and J.H. Moore 185 (1994) 297

Computational and simulation methods
Calculation of product branching ratios for the reaction of an ion with a molecule in a $^2\Pi$ electronic state, A.G. Wickham and D.C. Clary 185 (1994) 57
Experimental and computational investigation of the quadratic hyperpolarizability of a series of diaryls and polyaryls, M. Barzoukas, A. Fort, P. Boy, C. Combellas and A. Thiebault 185 (1994) 65
Modelling excimer formation in vinyl aromatic polymers, M.J. Carey and D. Phillips 185 (1994) 75
Rotational surprisals and energy disposal from statistical simulations of the crossed beam reaction $C(^3P)+NO\rightarrow CN(v)+O(^3P)$, E. Wallin, P.A. Elofson and L. Holmlid 185 (1994) 91
Tunneling trajectories of two-proton transfer, V.A. Benderskii, S.Yu. Grebenshchikov, D.E. Makarov and E.V. Vetoshkin 185 (1994) 101
Polaron-like variational solutions for low-lying vibronic states, L.F. Chibotaru and I.N. Kotov 185 (1994) 153
Network of strongly interacting atoms in liquid argon, G. Pálinkás and P. Jedlovszky 185 (1994) 173
Vibrational transition probabilities for the CO molecule trapped in an argon cluster: a semiclassical simulation, M.B. Sevryuk and G.D. Billing 185 (1994) 199
Fractal approach to the kinetics of an encounter pair between asymmetric reagents, M.C. Buján-Núñez and M.A. López-Quintela 185 (1994) 211
Improved sudden and adiabatic nuclei theories of atom–diatomic molecule scattering, C.-K. Zhang, T.-Q. Ren, W. Li and Y.-C. Zhang 185 (1994) 309
Molecular photoionization cross sections by the Lobatto technique. II. Core level photoionization, I. Wilhelmy and N. Rösch 185 (1994) 317
Quantum-chemical ab initio investigation of the two-step charge transfer process of hydrogen reaction: approach of reaction pathways via a hydrogen intermediate on Cu(100), An.M. Kuznetsov and W. Lorenz 185 (1994) 333

Molecular dynamics and scattering theory
Calculation of product branching ratios for the reaction of an ion with a molecule in a $^2\Pi$ electronic state, A.G. Wickham and D.C. Clary 185 (1994) 57
Chemiluminescent electron transfer reactions of C_{60} anion radical: energetics and spectral features, N. Gupta and K.S.V. Santhanam 185 (1994) 113
Quantum scattering on the Σ–Π intersection of potential energy surfaces, V.I. Osherov, L.V. Poluyanov, V.G. Ushakov and A.I. Voronin 185 (1994) 123
Improved sudden and adiabatic nuclei theories of atom–diatomic molecule scattering, C.-K. Zhang, T.-Q. Ren, W. Li and Y.-C. Zhang 185 (1994) 309

Experimental

Magnetic resonances
Pulsed-EPR on the photoexcited triplet state of C_{60} in fluid solution: electron transfer from end-capped quaterthiophene and C_{60}-radical anion formation, M. Bennati, A. Grupp, P. Bäuerle and M. Mehring 185 (1994) 221
Physical characterization of the state of motion of the phenalenyl spin probe in cation-exchanged faujasite zeolite supercages with pulsed EPR, D.C. Doetschman, D.W. Dwyer, J.D. Fox, C.K. Frederick, S. Scull, G.D. Thomas, S.G. Utterback and J. Wei 185 (1994) 343

Infrared spectroscopy
Aluminium, gallium and indium dihydrides. An IR matrix isolation and ab initio study, P. Pullumbi, C. Mijoule, L. Manceron and Y. Bouteiller 185 (1994) 13

Aluminium, gallium and indium trihydrides. An IR matrix isolation and ab initio study, P. Pullumbi, Y. Bouteiller, L. Manceron and C. Mijoule 185 (1994) 25
Infrared laser kinetic spectroscopy of the H_3^+ ion, M. Fehér, A. Rohrbacher and J.P. Maier 185 (1994) 357
Matrix isolation investigation of the vibrational spectroscopy and photochemistry of complexes of HCl and HBr with nitric oxide. Ab initio study of the NO:HCl complex structure, A. de Saxce, N. Sanna, A. Schriver and L. Schriver-Mazzuoli 185 (1994) 365

Visible and UV spectroscopy
Time-resolved spectroscopy of gaseous xenon excited in the vicinity of the first resonance line, A.V. Kanaev, T. Möller and P. Gürtler 185 (1994) 129
Triplet excitation migration for compound molecules in solid solutions, S.A. Bagnich 185 (1994) 229
Inhomogeneous spectral broadening in pentacene doped para-terphenyl crystals at high pressure and low temperature, B.J. Baer and E.L. Chronister 185 (1994) 385
Comment on "Photochemical reaction of 4-methyl-2-quinolinecarbonitrile with optically active (S)- or (R)-2-phenylpropionic acid. The magnetic-field and solvent effects and chiral-symmetry breaking", R. Nakagaki 185 (1994) 405

Fluorescence spectroscopy
Chemiluminescent electron transfer reactions of C_{60} anion radical: energetics and spectral features, N. Gupta and K.S.V. Santhanam 185 (1994) 113
Dual emission and double proton transfer in salicylic acid, D.D. Pant, H.C. Joshi, P.B. Bisht and H.B. Tripathi 185 (1994) 137
Inhomogeneous spectral broadening in pentacene doped para-terphenyl crystals at high pressure and low temperature, B.J. Baer and E.L. Chronister 185 (1994) 385
Experimental support for a novel compound motion model for the time-resolved fluorescence anisotropy decay of TMA-DPH in lipid vesicle bilayers, J.M. Muller, E.E. van Faassen and G. van Ginkel 185 (1994) 393

Electron impact spectroscopy
(e, 2e) Momentum spectroscopic study of the valence orbitals of hydrogen selenide, C.K. Subramaniam, M.A. Coplan, J.A. Tossell, J.H. Moore and K.T. Leung 185 (1994) 237
The lowest energy unoccupied molecular orbitals of the cyclopolysilanes: experimental and theoretical studies, J.A. Tossell, D.C. Winkler and J.H. Moore 185 (1994) 297

Laser methods
Photodissociation of ClNO in the A band, P. Felder and G.P. Morley 185 (1994) 145
The yield of $O_2(b\,^1\Sigma_g^+,\ v=0)$ produced by quenching of $O_2(A\,^3\Sigma_u^+,\ v=8)$ by O_2, G. Bednarek, R.P. Wayne, J. Wildt and E.H. Fink 185 (1994) 251
Infrared laser kinetic spectroscopy of the H_3^+ ion, M. Fehér, A. Rohrbacher and J.P. Maier 185 (1994) 357

Non-linear optical spectroscopy
Experimental and computational investigation of the quadratic hyperpolarizability of a series of diaryls and polyaryls, M. Barzoukas, A. Fort, P. Boy, C. Combellas and A. Thiebault 185 (1994) 65

Synchrotron spectroscopies
Time-resolved spectroscopy of gaseous xenon excited in the vicinity of the first resonance line, A.V. Kanaev, T. Möller and P. Gürtler 185 (1994) 129

Time-resolved experiments
Modelling excimer formation in vinyl aromatic polymers, M.J. Carey and D. Phillips 185 (1994) 75
Dual emission and double proton transfer in salicylic acid, D.D. Pant, H.C. Joshi, P.B. Bisht and H.B. Tripathi 185 (1994) 137
Pulsed-EPR on the photoexcited triplet state of C_{60} in fluid solution: electron transfer from end-capped quaterthiophene and C_{60}-radical anion formation, M. Bennati, A. Grupp, P. Bäuerle and M. Mehring 185 (1994) 221
Physical characterization of the state of motion of the phenalenyl spin probe in cation-exchanged faujasite zeolite supercages with pulsed EPR, D.C. Doetschman, D.W. Dwyer, J.D. Fox, C.K. Frederick, S. Scull, G.D. Thomas, S.G. Utterback and J. Wei 185 (1994) 343
Infrared laser kinetic spectroscopy of the H_3^+ ion, M. Fehér, A. Rohrbacher and J.P. Maier 185 (1994) 357

Mass spectrometry
Photodissociation of ClNO in the A band, P. Felder and G.P. Morley 185 (1994) 145

Objects

Bulk systems

Gases
Electron degradation and thermalization in SiH_4 gas, K. Kowari and B.D. Shizgal 185 (1994) 1
Time-resolved spectroscopy of gaseous xenon excited in the vicinity of the first resonance line, A.V. Kanaev, T. Möller and P. Gürtler 185 (1994) 129
The evolution of simple velocity averages of ions in gases in time-varying electric fields and static magnetic fields, L. Ferrari 185 (1994) 179
The yield of $O_2(b\,^1\Sigma_g^+,\ v=0)$ produced by quenching of $O_2(A\,^3\Sigma_u^+,\ v=8)$ by O_2, G. Bednarek, R.P. Wayne, J. Wildt and E.H. Fink 185 (1994) 251

Liquids neat
Network of strongly interacting atoms in liquid argon, G. Pálinkás and P. Jedlovszky 185 (1994) 173

Liquids mixtures and solutions
Experimental and computational investigation of the quadratic hyperpolarizability of a series of diaryls and polyaryls, M. Barzoukas, A. Fort, P. Boy, C. Combellas and A. Thiebault 185 (1994) 65
Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. IV. Stimulated polarization of nuclei in switched external magnetic field, A.M. Osintsev, P.A. Purtov and A.B. Doktorov 185 (1994) 281

Crystals
Matrix isolation investigation of the vibrational spectroscopy and photochemistry of complexes of HCl and HBr with nitric oxide. Ab initio study of the NO:HCl complex structure, A. de Saxce, N. Sanna, A. Schriver and L. Schriver-Mazzuoli 185 (1994) 365

–mixed
Inhomogeneous spectral broadening in pentacene doped para-terphenyl crystals at high pressure and low temperature, B.J. Baer and E.L. Chronister 185 (1994) 385

Glasses
Triplet excitation migration for compound molecules in solid solutions, S.A. Bagnich 185 (1994) 229

Liquid crystals
Experimental support for a novel compound motion model for the time-resolved fluorescence anisotropy decay of TMA-DPH in lipid vesicle bilayers, J.M. Muller, E.E. van Faassen and G. van Ginkel 185 (1994) 393

Metals and alloys
Aluminium, gallium and indium dihydrides. An IR matrix isolation and ab initio study, P. Pullumbi, C. Mijoule, L. Manceron and Y. Bouteiller 185 (1994) 13
Aluminium, gallium and indium trihydrides. An IR matrix isolation and ab initio study, P. Pullumbi, Y. Bouteiller, L. Manceron and C. Mijoule 185 (1994) 25

Biological systems
Experimental support for a novel compound motion model for the time-resolved fluorescence anisotropy decay of TMA-DPH in lipid vesicle bilayers, J.M. Muller, E.E. van Faassen and G. van Ginkel 185 (1994) 393

Microscopic systems

Atoms
Rotational surprisals and energy disposal from statistical simulations of the crossed beam reaction $C(^3P)+NO\rightarrow CN(v)+O(^3P)$, E. Wallin, P.A. Elofson and L. Holmlid 185 (1994) 91

Molecules (neutral and ionic)
Chemiluminescent electron transfer reactions of C_{60} anion radical: energetics and spectral features, N. Gupta and K.S.V. Santhanam 185 (1994) 113
A study of the ground and low-lying states of $MgC_2H_2^+$ and $MgC_2H_4^+$, M. Sodupe and C.W. Bauschlicher Jr. 185 (1994) 163
(e, 2e) Momentum spectroscopic study of the valence orbitals of hydrogen selenide, C.K. Subramaniam, M.A. Coplan, J.A. Tossell, J.H. Moore and K.T. Leung 185 (1994) 237

–diatomic
Ab initio CI study of the electronic spectrum of the interstellar free radical CP, J. Gu, R.J. Buenker and G. Hirsch 185 (1994) 39
Full configuration interaction calculations on Be_2, S. Evangelisti, G.L. Bendazzoli and L. Gagliardi 185 (1994) 47
Rotational surprisals and energy disposal from statistical simulations of the crossed beam reaction $C(^3P)+NO\rightarrow CN(v)+O(^3P)$, E. Wallin, P.A. Elofson and L. Holmlid 185 (1994) 91
Time-resolved spectroscopy of gaseous xenon excited in the vicinity of the first resonance line, A.V. Kanaev, T. Möller and P. Gürtler 185 (1994) 129
The yield of $O_2(b\,^1\Sigma_g^+,\ v=0)$ produced by quenching of $O_2(A\,^3\Sigma_u^+,\ v=8)$ by O_2, G. Bednarek, R.P. Wayne, J. Wildt and E.H. Fink 185 (1994) 251
Improved sudden and adiabatic nuclei theories of atom–diatomic molecule scattering, C.-K. Zhang, T.-Q. Ren, W. Li and Y.-C. Zhang 185 (1994) 309
Molecular photoionization cross sections by the Lobatto technique. II. Core level photoionization, I. Wilhelmy and N. Rösch 185 (1994) 317

–small polyatomics
Electron degradation and thermalization in SiH_4 gas, K. Kowari and B.D. Shizgal 185 (1994) 1
Photodissociation of ClNO in the A band, P. Felder and G.P. Morley 185 (1994) 145
A study of the ground and low-lying states of $MgC_2H_2^+$ and $MgC_2H_4^+$, M. Sodupe and C.W. Bauschlicher Jr. 185 (1994) 163
(e, 2e) Momentum spectroscopic study of the valence orbitals of hydrogen selenide, C.K. Subramaniam, M.A. Coplan, J.A. Tossell, J.H. Moore and K.T. Leung 185 (1994) 237
Semiclassical quantization of the spectroscopist's Hamiltonian for coupled vibrational modes, M. Joyeux 185 (1994) 263
The lowest energy unoccupied molecular orbitals of the cyclopolysilanes: experimental and theoretical studies, J.A. Tossell, D.C. Winkler and J.H. Moore 185 (1994) 297
Molecular photoionization cross sections by the Lobatto technique. II. Core level photoionization, I. Wilhelmy and N. Rösch 185 (1994) 317
Infrared laser kinetic spectroscopy of the H_3^+ ion, M. Fehér, A. Rohrbacher and J.P. Maier 185 (1994) 357

–aromatics
Pulsed-EPR on the photoexcited triplet state of C_{60} in fluid solution: electron transfer from end-capped quaterthiophene and C_{60}-radical anion formation, M. Bennati, A. Grupp, P. Bäuerle and M. Mehring 185 (1994) 221
Inhomogeneous spectral broadening in pentacene doped para-terphenyl crystals at high pressure and low temperature, B.J. Baer and E.L. Chronister 185 (1994) 385
Comment on "Photochemical reaction of 4-methyl-2-quinolinecarbonitrile with optically active (S)- or (R)-2-phenylpropionic acid. The magnetic-field and solvent effects and chiral-symmetry breaking", R. Nakagaki 185 (1994) 405

–other large
Experimental and computational investigation of the quadratic hyperpolarizability of a series of diaryls and polyaryls, M. Barzoukas, A. Fort, P. Boy, C. Combellas and A. Thiebault 185 (1994) 65

–polymeric and biological
Modelling excimer formation in vinyl aromatic polymers, M.J. Carey and D. Phillips 185 (1994) 75

Molecular aggregates
Polaron-like variational solutions for low-lying vibronic states, L.F. Chibotaru and I.N. Kotov 185 (1994) 153

–dimers
Tunneling trajectories of two-proton transfer, V.A. Benderskii, S.Yu. Grebenshchikov, D.E. Makarov and E.V. Vetoshkin 185 (1994) 101
Dual emission and double proton transfer in salicylic acid, D.D. Pant, H.C. Joshi, P.B. Bisht and H.B. Tripathi 185 (1994) 137

–clusters
Network of strongly interacting atoms in liquid argon, G. Pálinkás and P. Jedlovszky 185 (1994) 173
Vibrational transition probabilities for the CO molecule trapped in an argon cluster: a semiclassical simulation, M.B. Sevryuk and G.D. Billing 185 (1994) 199
Triplet excitation migration for compound molecules in solid solutions, S.A. Bagnich 185 (1994) 229

Quantum-chemical ab initio investigation of the two-step charge transfer process of hydrogen reaction: approach of reaction pathways via a hydrogen intermediate on Cu(100), An.M. Kuznetsov and W. Lorenz 185 (1994) 333

–complexes

Matrix isolation investigation of the vibrational spectroscopy and photochemistry of complexes of HCl and HBr with nitric oxide. Ab initio study of the NO:HCl complex structure, A. de Saxce, N. Sanna, A. Schriver and L. Schriver-Mazzuoli 185 (1994) 365

Free radicals (including hydronium and muonium)

Calculation of product branching ratios for the reaction of an ion with a molecule in a $^2\Pi$ electronic state, A.G. Wickham and D.C. Clary 185 (1994) 57

Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. IV. Stimulated polarization of nuclei in switched external magnetic field, A.M. Osintsev, P.A. Purtov and A.B. Doktorov 185 (1994) 281

Physical characterization of the state of motion of the phenalenyl spin probe in cation-exchanged faujasite zeolite supercages with pulsed EPR, D.C. Doetschman, D.W. Dwyer, J.D. Fox, C.K. Frederick, S. Scull, G.D. Thomas, S.G. Utterback and J. Wei 185 (1994) 343

Comment on "Photochemical reaction of 4-methyl-2-quinolinecarbonitrile with optically active (S)- or (R)-2-phenylpropionic acid. The magnetic-field and solvent effects and chiral-symmetry breaking", R. Nakagaki 185 (1994) 405

Ions and charge carriers

Electron degradation and thermalization in SiH_4 gas, K. Kowari and B.D. Shizgal 185 (1994) 1

Calculation of product branching ratios for the reaction of an ion with a molecule in a $^2\Pi$ electronic state, A.G. Wickham and D.C. Clary 185 (1994) 57

The evolution of simple velocity averages of ions in gases in time-varying electric fields and static magnetic fields, L. Ferrari 185 (1994) 179

Quantum-chemical ab initio investigation of the two-step charge transfer process of hydrogen reaction: approach of reaction pathways via a hydrogen intermediate on Cu(100), An.M. Kuznetsov and W. Lorenz 185 (1994) 333

Infrared laser kinetic spectroscopy of the H_3^+ ion, M. Fehér, A. Rohrbacher and J.P. Maier 185 (1994) 357

Phenomena

Molecular structure

Ab initio CI study of the electronic spectrum of the interstellar free radical CP, J. Gu, R.J. Buenker and G. Hirsch 185 (1994) 39

A study of the ground and low-lying states of $MgC_2H_2^+$ and $MgC_2H_4^+$, M. Sodupe and C.W. Bauschlicher Jr. 185 (1994) 163

Vibrations and rotations of molecules

Rotational surprisals and energy disposal from statistical simulations of the crossed beam reaction $C(^3P)+NO\rightarrow CN(v)+O(^3P)$, E. Wallin, P.A. Elofson and L. Holmlid 185 (1994) 91

Semiclassical quantization of the spectroscopist's Hamiltonian for coupled vibrational modes, M. Joyeux 185 (1994) 263

Improved sudden and adiabatic nuclei theories of atom–diatomic molecule scattering, C.-K. Zhang, T.-Q. Ren, W. Li and Y.-C. Zhang 185 (1994) 309

Electronic structure and states

Ab initio CI study of the electronic spectrum of the interstellar free radical CP, J. Gu, R.J. Buenker and G. Hirsch 185 (1994) 39

Full configuration interaction calculations on Be_2, S. Evangelisti, G.L. Bendazzoli and L. Gagliardi 185 (1994) 47

A study of the ground and low-lying states of $MgC_2H_2^+$ and $MgC_2H_4^+$, M. Sodupe and C.W. Bauschlicher Jr. 185 (1994) 163

(e, 2e) Momentum spectroscopic study of the valence orbitals of hydrogen selenide, C.K. Subramaniam, M.A. Coplan, J.A. Tossell, J.H. Moore and K.T. Leung 185 (1994) 237

The lowest energy unoccupied molecular orbitals of the cyclopolysilanes: experimental and theoretical studies, J.A. Tossell, D.C. Winkler and J.H. Moore 185 (1994) 297

Quantum-chemical ab initio investigation of the two-step charge transfer process of hydrogen reaction: approach of reaction pathways via a hydrogen intermediate on Cu(100), An.M. Kuznetsov and W. Lorenz 185 (1994) 333

Electric and magnetic properties

The evolution of simple velocity averages of ions in gases in time-varying electric fields and static magnetic fields, L. Ferrari 185 (1994) 179

Spin splittings

Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. IV. Stimulated polarization of nuclei in switched external magnetic field, A.M. Osintsev, P.A. Purtov and A.B. Doktorov 185 (1994) 281

Molecular interactions

Network of strongly interacting atoms in liquid argon, G. Pálinkás and P. Jedlovszky 185 (1994) 173

Matrix isolation investigation of the vibrational spectroscopy and photochemistry of complexes of HCl and HBr with nitric oxide. Ab initio study of the NO:HCl complex structure, A. de Saxce, N. Sanna, A. Schriver and L. Schriver-Mazzuoli 185 (1994) 365

Inhomogeneous spectral broadening in pentacene doped para-terphenyl crystals at high pressure and low temperature, B.J. Baer and E.L. Chronister 185 (1994) 385

Spectral bandshapes and intensities

Ab initio CI study of the electronic spectrum of the interstellar free radical CP, J. Gu, R.J. Buenker and G. Hirsch 185 (1994) 39

Coupling of electronic and nuclear motion

Quantum scattering on the Σ–Π intersection of potential energy surfaces, V.I. Osherov, L.V. Poluyanov, V.G. Ushakov and A.I. Voronin 185 (1994) 123

Energy transfer processes

Electron degradation and thermalization in SiH_4 gas, K. Kowari and B.D. Shizgal 185 (1994) 1

Quantum scattering on the Σ–Π intersection of potential energy surfaces, V.I. Osherov, L.V. Poluyanov, V.G. Ushakov and A.I. Voronin 185 (1994) 123

Time-resolved spectroscopy of gaseous xenon excited in the vicinity of the first resonance line, A.V. Kanaev, T. Möller and P. Gürtler 185 (1994) 129
Vibrational transition probabilities for the CO molecule trapped in an argon cluster: a semiclassical simulation, M.B. Sevryuk and G.D. Billing 185 (1994) 199
Triplet excitation migration for compound molecules in solid solutions, S.A. Bagnich 185 (1994) 229
The yield of $O_2(b\,^1\Sigma_g^+,\ v=0)$ produced by quenching of $O_2(A\,^3\Sigma_u^+,\ v=8)$ by O_2, G. Bednarek, R.P. Wayne, J. Wildt and E.H. Fink 185 (1994) 251

Molecular photophysical processes
Modelling excimer formation in vinyl aromatic polymers, M.J. Carey and D. Phillips 185 (1994) 75
Chemiluminescent electron transfer reactions of C_{60} anion radical: energetics and spectral features, N. Gupta and K.S.V. Santhanam 185 (1994) 113
Dual emission and double proton transfer in salicylic acid, D.D. Pant, H.C. Joshi, P.B. Bisht and H.B. Tripathi 185 (1994) 137
Pulsed-EPR on the photoexcited triplet state of C_{60} in fluid solution: electron transfer from end-capped quaterthiophene and C_{60}-radical anion formation, M. Bennati, A. Grupp, P. Bäuerle and M. Mehring 185 (1994) 221
Molecular photoionization cross sections by the Lobatto technique. II. Core level photoionization, I. Wilhelmy and N. Rösch 185 (1994) 317

Intramolecular dynamics
Polaron-like variational solutions for low-lying vibronic states, L.F. Chibotaru and I.N. Kotov 185 (1994) 153

Luminescence spectra, yields and lifetimes
Dual emission and double proton transfer in salicylic acid, D.D. Pant, H.C. Joshi, P.B. Bisht and H.B. Tripathi 185 (1994) 137

Coherence loss processes
Physical characterization of the state of motion of the phenalenyl spin probe in cation-exchanged faujasite zeolite supercages with pulsed EPR, D.C. Doetschman, D.W. Dwyer, J.D. Fox, C.K. Frederick, S. Scull, G.D. Thomas, S.G. Utterback and J. Wei 185 (1994) 343

Non-linear responses (including optical)
Experimental and computational investigation of the quadratic hyperpolarizability of a series of diaryls and polyaryls, M. Barzoukas, A. Fort, P. Boy, C. Combellas and A. Thiebault 185 (1994) 65

Reactions (including dissociation)

–gas phase
Calculation of product branching ratios for the reaction of an ion with a molecule in a $^2\Pi$ electronic state, A.G. Wickham and D.C. Clary 185 (1994) 57
Rotational surprisals and energy disposal from statistical simulations of the crossed beam reaction $C(^3P)+NO\rightarrow CN(v)+O(^3P)$, E. Wallin, P.A. Elofson and L. Holmlid 185 (1994) 91
Photodissociation of ClNO in the A band, P. Felder and G.P. Morley 185 (1994) 145

–condensed phase
Fractal approach to the kinetics of an encounter pair between asymmetric reagents, M.C. Buján-Núñez and M.A. López-Quintela 185 (1994) 211

–photochemical
Photodissociation of ClNO in the A band, P. Felder and G.P. Morley 185 (1994) 145
Theory of geminate recombination of radical pairs with instantaneously changing spin Hamiltonian. IV. Stimulated polarization of nuclei in switched external magnetic field, A.M. Osintsev, P.A. Purtov and A.B. Doktorov 185 (1994) 281
Matrix isolation investigation of the vibrational spectroscopy and photochemistry of complexes of HCl and HBr with nitric oxide. Ab initio study of the NO:HCl complex structure, A. de Saxce, N. Sanna, A. Schriver and L. Schriver-Mazzuoli 185 (1994) 365
Comment on "Photochemical reaction of 4-methyl-2-quinolinecarbonitrile with optically active (S)- or (R)-2-phenylpropionic acid. The magnetic-field and solvent effects and chiral-symmetry breaking", R. Nakagaki 185 (1994) 405

Tunneling
Tunneling trajectories of two-proton transfer, V.A. Benderskii, S.Yu. Grebenshchikov, D.E. Makarov and E.V. Vetoshkin 185 (1994) 101

Electron transfer
Chemiluminescent electron transfer reactions of C_{60} anion radical: energetics and spectral features, N. Gupta and K.S.V. Santhanam 185 (1994) 113
Pulsed-EPR on the photoexcited triplet state of C_{60} in fluid solution: electron transfer from end-capped quaterthiophene and C_{60}-radical anion formation, M. Bennati, A. Grupp, P. Bäuerle and M. Mehring 185 (1994) 221

Ionization (including Rydberg states)
Molecular photoionization cross sections by the Lobatto technique. II. Core level photoionization, I. Wilhelmy and N. Rösch 185 (1994) 317

Molecular motion (including diffusive)
Physical characterization of the state of motion of the phenalenyl spin probe in cation-exchanged faujasite zeolite supercages with pulsed EPR, D.C. Doetschman, D.W. Dwyer, J.D. Fox, C.K. Frederick, S. Scull, G.D. Thomas, S.G. Utterback and J. Wei 185 (1994) 343
Experimental support for a novel compound motion model for the time-resolved fluorescence anisotropy decay of TMA-DPH in lipid vesicle bilayers, J.M. Muller, E.E. van Faassen and G. van Ginkel 185 (1994) 393

Thermodynamic and transport properties
The evolution of simple velocity averages of ions in gases in time-varying electric fields and static magnetic fields, L. Ferrari 185 (1994) 179

Structure of solids and liquids
Network of strongly interacting atoms in liquid argon, G. Pálinkás and P. Jedlovszky 185 (1994) 173
Experimental support for a novel compound motion model for the time-resolved fluorescence anisotropy decay of TMA-DPH in lipid vesicle bilayers, J.M. Muller, E.E. van Faassen and G. van Ginkel 185 (1994) 393